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# Effect of interface state continuum on the forward (I–V) characteristics of metal-semiconductor contacts with thin interfacial layer

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**Abstract** : The effect of interface state continuum on the forward current-voltage characteristics of metal-semiconductor contact has been examined. It is observed that with the increase of the density of interface state continuum, the nonlinearity in the characteristics begins at lower voltages where the current increases The increase of current is due to quantum mechanical tunneling of electrons between the enhanced interface states and the metal, so as to provide additional current paths However, at higher voltages, the current decreases with the enhanced interface state density due to the increment on the part of the applied voltage drop across the interfacial layer For a particular density of interface state, the nonlinearity in the characteristics begins at lower voltages if the interaction rate of the interface states with the majority carriers is much larger than that with the minority carriers.

**Keywords** : Metal-semiconductor contact, interface state continuum, (I–V) characteristics

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## 1. Introduction

Although the performance and reliability of devices based on metal-semiconductor Schottky contact depend on the energy and density of interface states, little efforts have been done to investigate the effect of these states on Schottky (I–V) characteristics. Barret and Vapaille [1,2] in their theoretical work of characterization of these states, considered the interface state spectra as a set of discrete levels or narrow bands sparsely distributed within semiconductor band gap. Later on, this concept was modified by Muret and Deneuville [3] with the assumption that the distribution of the interface states within the band gap can be fitted by several localized rectangular bands. Recently, Chattopadhayay [4] took the case of discrete localized states to study their effect on the (I–V) behaviour of metal-semiconductor contacts.

However, experimentally it is found that for almost all MIS tunneling devices, the interface states are distributed in a wide continuum rather than in a few discrete levels in the semiconductor band gap [5,6]. Therefore, the distribution of the interface states for metal-semiconductor Schottky contacts can still be expected to be a continuum. In this paper, the effect of the interface state continuum on the forward (I–V) characteristics of metal-semiconductor contacts has been reported.

## 2. Theory

Figure 1 represents the energy band diagram of a forward biased metal-*n* type semiconductor contact with a thin interfacial layer. Here $\phi_m$ is the work function of the metal; $\chi$, the electron affinity of the semiconductor; $\psi_s$, the semiconductor surface potential; $\delta$, the thickness of the interfacial layer; $\Delta$, the voltage drop across the interfacial layer and

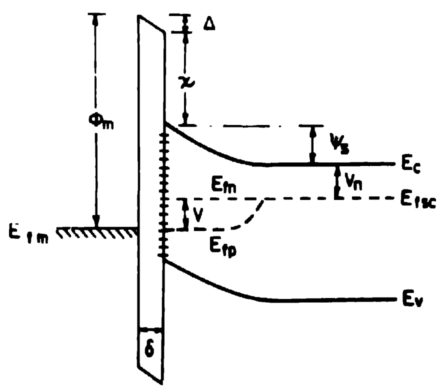


**Figure 1.** Energy band diagram of a forward biased metal-*n* type semiconductor contact with a thin interfacial layer.

$V_n$, the depth of the Fermi level below the conduction band edge in the bulk semiconductor. $E_{fn}$ and $E_{fp}$ are the respective quasi-Fermi levels for electrons and holes in the semiconductor at a forward bias voltage $V$ applied to the junction. Applied voltage $V$ consists of two components : $V = V_i + V_s$, where $V_i$ is the part of the applied voltage drop across the interfacial layer and $V_s$ that across the semiconductor space charge region.

Considering the energy band diagram, the voltage drop across the interfacial layer can be written as

$$\Delta = \phi_m - \chi - \psi_s - V_n - V. \tag{1}$$

The voltage drop across the interfacial layer can also be obtained by using charge neutrality condition and Gauss law. Thus,

$$\Delta = \frac{\delta}{\varepsilon_i}\left(Q_{sc} + Q_{it} + Q_f\right), \tag{2}$$

where $Q_{sc}$ is the semiconductor space charge density; $Q_{it}$, the interface trapped charge density and $Q_f$, the fixed charge density in the interfacial layer.

Taking the case of the interface state continuum throughout the band gap, the net charge density trapped in the interface states is given by [7]

$$Q_{it}(V_s) = -q\int_{E_v}^{E_c}\left[D_{it}^{a}(E_t) + D_{it}^{d}(E_t)\right]f_{it}(E_t,V_s)dE_t + q\int_{E_v}^{E_c} D_{it}^{d}(E_t)dE_t, \quad (3)$$

where $D_{it}^{a}(E_t)$ and $D_{it}^{d}(E_t)$ are the densities of acceptor and donor types of interface states at the energy level $E_t$, and $D_{it}(E_{it}) = D_{it}^{a}(E_t)+D_{it}^{d}(E_t)$. The occupation function $f_{it}(E_t,V_s)$ is assumed to be indistinguishable for both acceptor and donor types of the interface states.

The occupation function of the interface state is obtained using the Shockley-Read-Hall statistics and considering the charge exchanges between metal and interface states [8,9]. Thus,

$$f_{it}(E_t,V_s) = \frac{c_n n_s + c_p p_1(E_t) + f_m(E_t)/\tau_t}{c_n[n_s + n_1(E_t)] + c_p[p_s + p_1(E_t)] + 1/\tau_t}, \quad (4)$$

where $c_n$ and $c_p$ are the average capture rates of the interface states for electrons and holes; $n_s$ and $p_s$ are the quasi-thermal equilibrium densities of electrons and holes at the semiconductor surface; $n_1$ and $p_1$ are the densities of electrons and holes if their quasi-Fermi levels were coincident with trap energy level $E_t$; $f_m(E_t)$ is the probability of occupancy of state $E_t$ by the metal electron; $\tau_t$ is the electron tunneling time constant between the interface states and the metal conduction band.

Further,

$$n_s = n_i \exp[(E_{fn} - E_i)/kT], \quad (5a)$$

$$p_s = n_i \exp[(E_i - E_{fp})/kT], \quad (5b)$$

$$n_1(E_t) = n_i \exp[(E_t - E_i)/kT], \quad (5c)$$

$$p_1(E_t) = n_i \exp[(E_i - E_t)/kT], \quad (5d)$$

where $E_i$ is the intrinsic Fermi level of the semiconductor and $n_i$ is the intrinsic carrier concentration.

Since the quasi-Fermi level of minority carriers in the semiconductor is aligned with that of the metal at the interface, we can write

$$f_m(E_t) = \frac{1}{1 + \exp[(E_t - E_{fp})/kT]} = \frac{p_1(E_t)}{p_s + p_1(E_t)}. \quad (6)$$

With this substitution, eq. (4) becomes

$$f_{it}(E_t,V_s) = \frac{c_n n_s + c'_p p_1(E_t)}{c_n[n_s + n_1(E_t)] + c'_p[p_s + p_1(E_t)]}, \quad (7)$$

where $$c'_p = c_p + \frac{1}{\tau_t[p_s + p_1(E_t)]}.$$

Taking $c'_p / c_n = \alpha$, a parameter specifying the controllability of minority carriers on the occupancy of the interface state continuum, eq. (7) becomes

$$f_{it}(E_t, V_s) = \frac{n_s + \alpha p_1(E_t)}{n_s + n_1(E_t) + \alpha[p_s + p_1(E_t)]}. \tag{8}$$

Usually, the $(J-V)$ characteristics of most metal-semiconductor contacts are characterized by thermionic emission theory. Thus assuming interfacial layer-thermionic emission theory [10] the $(J-V)$ relation for these metal-semiconductor contacts can be written as

$$J = A^* T^2 \theta_n \exp\left[-\frac{q}{kT}(\psi_s + V_n)\right] \qquad \text{for } V > \frac{3kT}{q}, \tag{9}$$

where $A^*$ is the effective Richardson constant; $T$, the absolute temperature and $\theta_n$ is the transmission coefficient across the interfacial layer.

The transmission coefficient $\theta_n$ may be approximately expressed as [11]

$$\theta_n = \exp(-\chi_e^{1/2}\delta), \tag{10}$$

where $\chi_e = \frac{2}{\hbar}(2m_n\chi_e)^{1/2}$ is assumed to be independent of the applied voltage; $m_n$, the effective tunneling mass of electrons; and $\chi_e$ is the effective barrier height presented by the interfacial layer.

The voltage dependence of surface potential $\psi_s$ can be obtained numerically from eqs. (1–3). The values of $\psi_s$ thus calculated, can be used to obtain (J–V) characteristics of metal-semiconductor contact from eq. (9).

## 3. Discussion

The study has been carried out on any arbitrary metal/$n$-type Si contact where the metal has the work function 5.0 eV, like Co. The occupation function $f_{it}(E_t, V_s)$ of the interface state continuum within the band gap has been calculated with the help of eq. (8) The parameters used here are $\phi_m = 5.0$ eV, $\chi = 4.05$ eV, $N_d = 10^{16}$ cm$^{-3}$, $N_f = 5 \times 10^{11}$ cm$^{-2}$, $E_g = 1.12$ eV, $\delta = 10$ Å, $\varepsilon_s = 11.9$, $\varepsilon_i = 3.9$ and $\alpha = 0.01$. The occupation function thus obtained, is used to get interface trapped charge density $Q_{it}$ from eq. (3). Here, the interface states are assumed to be of donor nature and uniformly distributed throughout the semiconductor band gap.

Considering the interfacial layer to be of oxide layer and with $Q_{sc} = (2q\varepsilon_s N_d \psi_s)^{1/2}$ and $Q_f = qN_f$, $N_f$ being the density of fixed charges in the oxide layer, the values of $\psi_s$ have been calculated for different values of $V$ for a given interface state density from eqs (1) and (2) by a self-consistent iteration method. Plots of $\psi_s$ *vs* $V$ with interface state density as parameter are shown in Figure 2.

As desired by Card and Rhoderick [11], the band structure of the interfacial films formed in metal-semiconductor contacts does not resemble that of bulk $SiO_2$ even if one consider the film of thickness 26 Å; so it is unreasonable to use a value of $\chi_e$ of 3.15 eV obtained by William [12] in the case of thick film MOS devices. Card and Rhoderick calculated the effective transmission coefficients for oxide films of thickness from 8 Å to 26 Å. which have been used here in obtaining (J–V) characteristics of metal-semiconductor contacts.

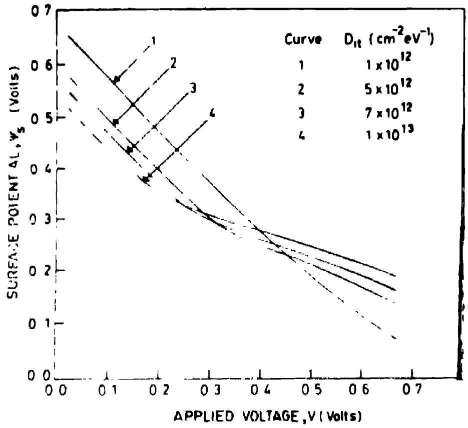


**Figure 2.** Voltage dependence of the surface potential $\psi_s$ at different values of the density of interface state continuum

The forward (J–V) characteristics of metal-semiconductor contact with interface state density as parameter are shown in Figure 3. The curve corresponding to $D_{it} = 0$ represents the ideal characteristic for which the logarithmic variation of current with voltage is linear. With the presence of the interface state continuum within the band gap, the

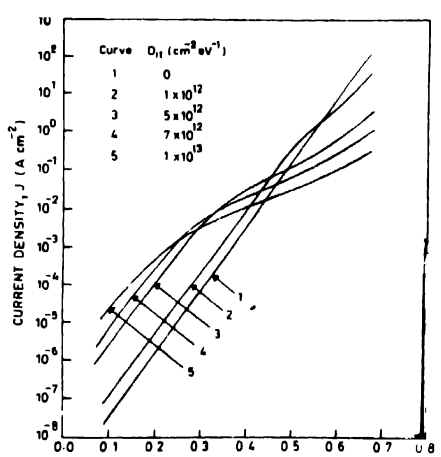


**Figure 3.** Effect of the density of interface state continuum on the forward (J–V) characteristics of metal-semiconductor contact.

variation of current with voltage becomes nonlinear. From Figure 3, it is clear that the nonlinearity in the characteristics begins at lower voltages as the density of interface state continuum increases. At lower voltages, the current has been found to increase with the increase of the density of interface state continuum. This can be understood with quantum mechanical tunneling of electrons between the enchanced interface states and the metal, which provides additional current paths. However, at higher voltages, the current decreases with the increase of the density of interface state continuum. This is due to the increment on the part of the applied voltage drop across the interfacial layer at higher voltages. Figure 4

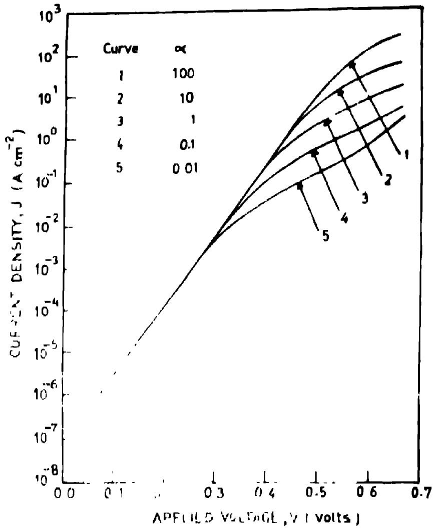


**Figure 4.** Effect of $\alpha$ on the forward (J–V) characteristics of metal-semiconductor contact for a typical value of $D_{it}(E_t) = 5 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$

shows the effect of $\alpha$ (a parameter specifying the controllability of minority carriers on the occupancy of interface state continuum) on the forward (J–V) characteristics of metal-semiconductor contact for a typical value of $D_{it}(E_t) = 5 \times 10^{12}$ cm$^{-2}$ eV$^{-1}$. It is seen that the nonlinearity in the characteristics begins at lower voltages if the interaction rate of the interface states with the majority carriers is much larger than that with the minority carriers.

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